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A numerical study on the flow characteristics in the mixing region of the catalytic combustor

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Abstract

Catalytic combustion is usually accomplished by a chemical reaction at the catalyst surface. Therefore, it is important that the fuel and air stream be well mixed and supplied uniformly. In this study, a perforated plate is used to enhance the mixing and flow uniformity for stable catalytic combustion. Also, a numerical simulation is performed to investigate the variation of flow characteristics according to various parameters. The results show that the uniformity of mixing and flow can be effectively improved for most of the cases by using a well-designed perforated plate.

Keywords: Catalytic combustor; Flow characteristics; Flow uniformity; Numerical study

1. Introduction

Since conventional burners have been used for a long time, well established technologies about their design and construction are available. Conventional burners are therefore very well optimized. However, it is difficult to control emissions such as NOx, UHC, and CO by using conventional burners, especially NOx emissions [1]. NOx emissions can be reduced by simply reducing the flame temperature, but limitations arise due to flame instability, pressure pulsations, and poor combustion efficiency (emissions of CO and UHC) [2]. In contrast, catalytic combustion can be achieved by a chemical reaction between the fuel and oxidizer at the catalyst surface, this type of com-bustion is different from the conventional one. Also, catalytic combustion requires neither a flame nor an ignition source like a spark or pilot flame. Fur-thermore, it is not bounded by flammability limits and is not penalized by the severity of the conditions within a flame. Catalytic combustion generally proceeds at a lower temperature than the conventional combustion. This results a decrease of the thermal NOx emission. Catalytic combustion is, therefore, an alternate form of conventional combustion, which has the potential to be a cleaner combustion process [3]. For this reason, catalytic combustion has been developed for application to gas turbine [2, 4-6]. Also, in fuel cell power systems, the com-bustor supplies high temperature mixture gases and heat needed by the reformer, by using the off-gas of the anode which includes a high condition and local concentrations of H_2O and CO_2. In this case, since a combustor needs to operate in a very fuel lean avoid heating to the reformer, a catalytic combustor is usually used.

Notwithstanding these advantages, the commercial application of catalytic combustion has been delayed due to the inability to develop catalysts that have the required stability and durability [4]. Especially, the durability problem of the catalyst and substrate is an important issue. As the catalytic reaction occurs, the catalyst surface reaction becomes diffusion limited,

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and at this point, the substrate temperature approaches the adiabatic com-bustion temperature of the fuel/air mixture. This results in thermal sintering of the support surface area, thermal sintering and vaporization of the active components such as noble metals, and thermal shock fracturing of ceramic supports. Therefore, it is important that the fuel and air streams are well mixed and supplied uniformly prior to the combustion region. If the flow is maldistributed, a hot spot may occur that can lead to the subsequent damage of the catalyst and substrate [3].

To enhance mixing and flow uniformity, a static mixer has been used for many cases of catalytic combustion [7]. Although the static mixer provides good mixing and flow uniformity, it is an inappropriate device because it needs to be long in a system that requires a compact configuration. Berg et al. [8] used a tee-type ejector at the mixing section and obtained a deviation of gas concentration of less than 1%. However, it can be successfully applied to the system without any space limitation because it requires an increase of the distance between the mixing point and the inlet of the catalyst to enhance the mixing quality. Also, although several studies on the enhancement of flow uniformity have been reported in the literature [9, 10], they have not achieved a satisfactory level of flow and mixing characteristics required for the catalytic combustor.

Consequently, in this study, a perforated plate is used to supply a uniform flow stream prior to the catalytic combustion region. A mathematical model for the prediction of flow and mixing characteristics in the mixing region of the catalytic combustor adopted in fuel cell power plant systems is suggested by using numerical methods. After verifying the results by comparing results with experimental data, we performed comprehensive numerical simulation to investigate the variation of flow characteristics by changing such various parameters as inlet configuration, volume flow rate, porous area and the number of the perforated plates used. Under each condition, the uniformity of the flow stream at the entrance of the catalyst section was evaluated and compared.

2. Numerical model

Numerical analysis of the mixing region of the catalytic combustor has been carried out by using the CFD code FIRE v8.4 [11], which is based on the finite volume approach. The solution algorithm employed enables flexibility in the usage of any unstructured grids including grids consisting of polyhedral control volumes. A state-of-the-art turbulence model has been implemented for accurate calculations of turbulent flows. The upwind scheme and turbulence model of standard high-*Re*-number $k-\varepsilon$ model have been applied in this study.

2.1 Governing equations

The local value of velocity and turbulent quantities can be represented by the following expression:

• Continuity equation

$$\frac{\partial(\rho U_j)}{\partial x_j}=0 \tag{1}$$

• Momentum equation

$$\rho U_i\left(\frac{\partial U_i}{\partial x_j}\right)=\rho g_i-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\mu\left\{\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}-\frac{2}{3}\left(\frac{\partial U_k}{\partial x_k}\right)\delta_{ij}\right\}\right] \tag{2}$$

• Turbulence model: $k-\varepsilon$ model

$$\rho\frac{\partial k}{\partial t}+\rho U_j\frac{\partial k}{\partial x_j}=\mathrm{P+G}-\varepsilon+\frac{\partial}{\partial x_j}\left(\mu+\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right) \tag{3}$$

$$\rho\frac{\partial \varepsilon}{\partial t}=\left(\mathrm{C}_{\varepsilon 1}\mathrm{P}+\mathrm{C}_{\varepsilon 3}\mathrm{G}+\mathrm{C}_{\varepsilon 4}k\frac{\partial U_k}{\partial x_k}-C_{\varepsilon 2}\varepsilon\right)\frac{\varepsilon}{k}+\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) \tag{4}$$

2.2 Boundary conditions

While the mass flow rate is specified at the inlet of the catalytic combustor, the no-slip condition is used at the wall. The outlet condition of the catalytic combustor is assigned the atmospheric pressure (101,315 Pa). The tube friction option of the porosity module in FIRE is applicable for flow through the catalytic monolith, because the empirical data of the

Table 1. The coefficients of $k-\varepsilon$ equation.

$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	$C_{\varepsilon 3}$	$C_{\varepsilon 4}$	σ_k	σ_ε
1.44	1.92	0.8	0.33	1	1.3

pressure drop of the catalyst is not available. In this module, the pressure drop is calculated by the wall friction within catalyst monolith. The mean hydraulic diameter of the catalyst tube is 0.001 m, corresponding to about 400 cpsi.

2.3 Model configuration and computational grid

Fig. 1 shows the perforated plate used in this study in order to achieve flow uniformity. It has different porous areas of 5.7, 10.6 and 15.2%, respectively, and thickness of 1mm. The mesh system used in this work is illustrated in Fig. 2.

To evaluate the effects of the perforated plates on the flow and mixing characteristics in the mixing

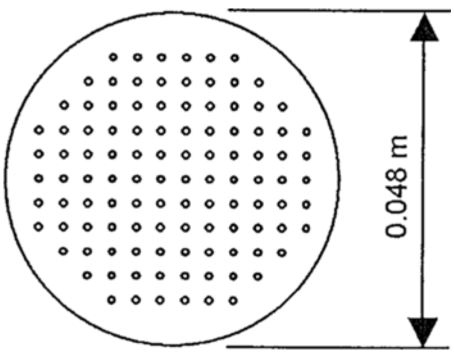


Fig. 1. Schematic of the perforated plate used in this work.

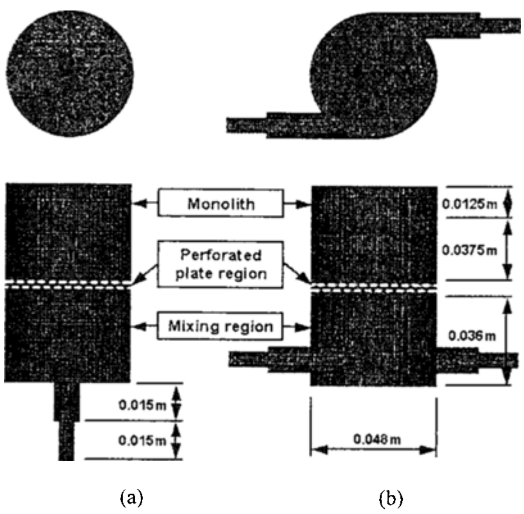


Fig. 2. The computational domain and dimension of (a) upward and (b) swirl type injection.

region, two different types of inlet geometry, such as upward and swirl types, are used because they can supply an intensive flow in order to simulate a terrible operating condition of the catalytic combustor. The computational domain is discretized by using an element size of 0.7 mm for the mixing and honeycomb monolith region. For the regions of the perforated plates, an element size of 0.025 mm~0.035 mm was used to fit the perforated hole of the plate. Both upward and swirl types contain about 450,000 - 750,000 cells for each case.

2.4 Estimation of the flow uniformity

To estimate the flow uniformity, the standard deviation expressed in Eq. (5) is used. Standard deviation is the most common measure of dispersion, measuring how widely spread the values of a data set are. If the data points are all close to the mean, then the standard deviation is close to zero. If many data points are far from the mean, then the standard deviation is far from zero. If all the data values are equal, then the standard deviation is zero. It is defined by the following expression:

$$\sigma = \sqrt{\frac{\sum\left(U-\bar{U}\right)^2}{n-1}} \tag{5}$$

where, $\bar{U}$ is the average velocity and n is the number of the sampling data.

3. Experimental measurement

For verification of the simulation results, the experimental work to measure the exit velocity of the catalytic combustor was performed for the non-reacting case. As shown in Fig. 3, the velocity profile at the outlet of honeycomb monolith was measured by using a hot-wire anemometer for 20 cells in the measurement line. In this study, because the systems have axisymmetric characteristics only one measure-

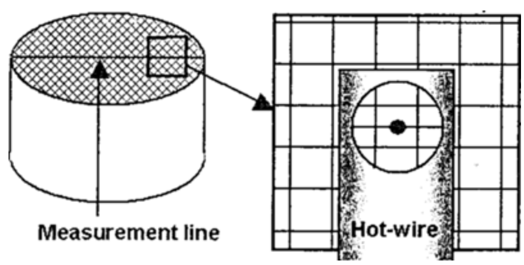


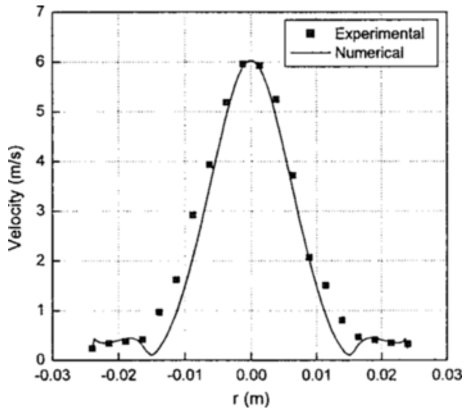
Fig. 3. Measurement line of the velocity at honeycomb monolith outlet.

ment line was chosen and the experimental velocity data were used as benchmarking data for the validation of the numerical results.

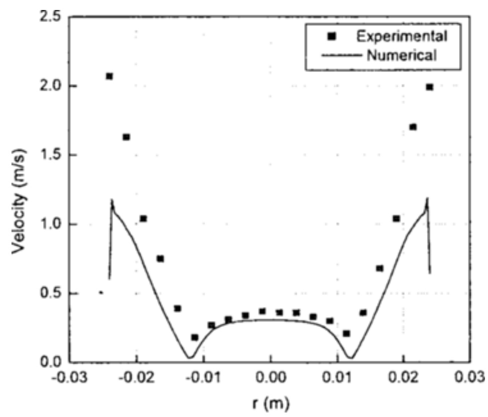
4. Results and discussion

Figs. 4(a) and 4(b) show the experimental and simulation results for the upward and swirl type models for the case of no perforated plate, respectively, at the honeycomb outlet for volume flow rate of 50 lpm, and Fig. 4(c) presents the three-dimensional simulation results at that cross-section. The simulation results of the upward type are in good agreement with the corresponding experimental results. Also, the simulation results of the swirl type show a similar tendency to the experimental results on the whole, although a difference exists between the experimental and simulation results in the vicinity of the side wall. In the upward type model, it can be found that the flow is concentrated in the center region of the combustor because of the inlet configuration, and the maximum velocity reaches about 6 m/s. In this case, since the residence time of the fuel in the catalyst section is of short duration, it is expected that most of the fuel cannot react with precious metals in the catalyst section.

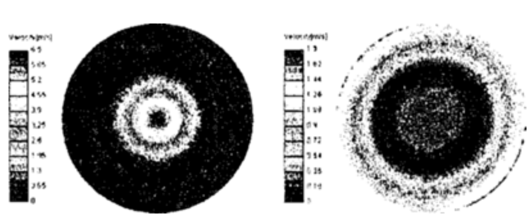
Consequently, it is expected that a high velocity flow concentrated in the center can result in fuel slip. Also, in the swirl type model, the flow is concentrated



(a)

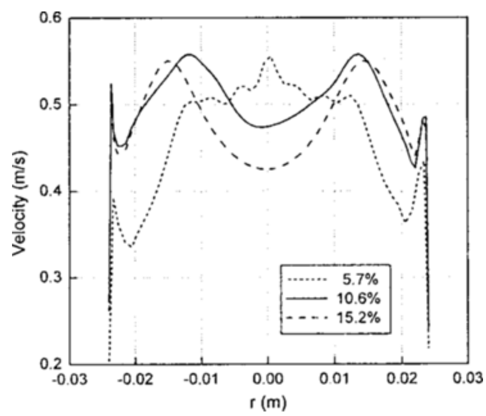


(b)

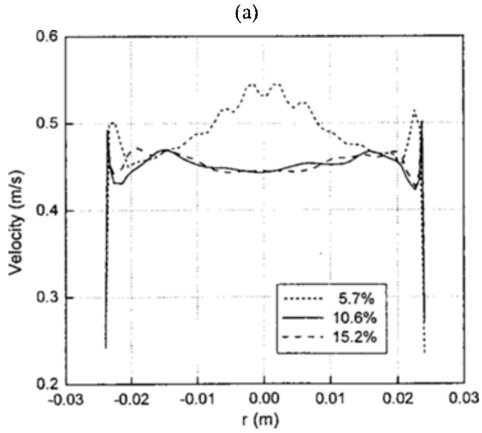


(c)

Fig. 4. Comparison of experimental and simulation results: (a) upward type, (b) swirl type, and (c) velocity contours at the honeycomb monolith outlet.



(a)



(b)

Fig. 5. Effect of porous area of the perforated plates on the velocity profile: (a) upward type and (b) swirl type.

Table 2. Standard deviation by variation of the porous area.

	Upward type	Swirl type
5.7 %	0.063	0.028
10.6 %	0.034	0.012
15.2 %	0.042	0.013

in the wall region of the catalytic combustor because of the swirl motion produced by the inlet configuration of the swirl type, and the velocity at the center is very low. If the flow has a low velocity in the center as shown in Fig. 4(b), a hot spot may occur at this region. Subsequently, this hot spot could damage the catalyst and substrate. This result reflects the three-dimensional flow patterns shown in Fig. 4(c). The standard deviation of this non-perforated plate case is 2.040 and 0.328 for the upward and swirl types, respectively.

To investigate the most appropriate proportion of the porous area in a perforated plate, the effects of the variation of the porous area on velocity profile for the catalytic combustor are investigated by using the two-perforated plates at the volume flow rate of 50 lpm. The simulation results for the cases of porous area of 5.7, 10.6, and 15.2%, respectively, are presented in Fig. 5. In both upward and swirl types, the velocity profile for the case of 10.6% porous area is more uniform than the case with 5.7 and 15.2% porous area. Also, it can be found that the swirl type model is more effective than upward type model with respect to flow uniformity. This is because the introduced flow is concentrated at the center region in the upward type, while swirl type disperses the flow to the wall. Therefore, the perforated plate with the porous area of 10.6% is adopted in the simulation model after this. Table 2 shows the standard deviation qualitatively for each case of the porous area.

Figs. 6(a) and 6(b) show the effects of the number of perforated plates used on the velocity profile at the volume flow rate of 50 lpm. It can be observed that there exists a severe maldistribution when the perforated plate is not used. The velocity profile, however, gradually becomes more uniform as the number of perforated plate increases. When one perforated plate of the upward type is used, flow is still concentrated in the center region although the maximum velocity is reduced to about one-third of that of the model without a perforated plate. As the number of the perforated plates increases by more

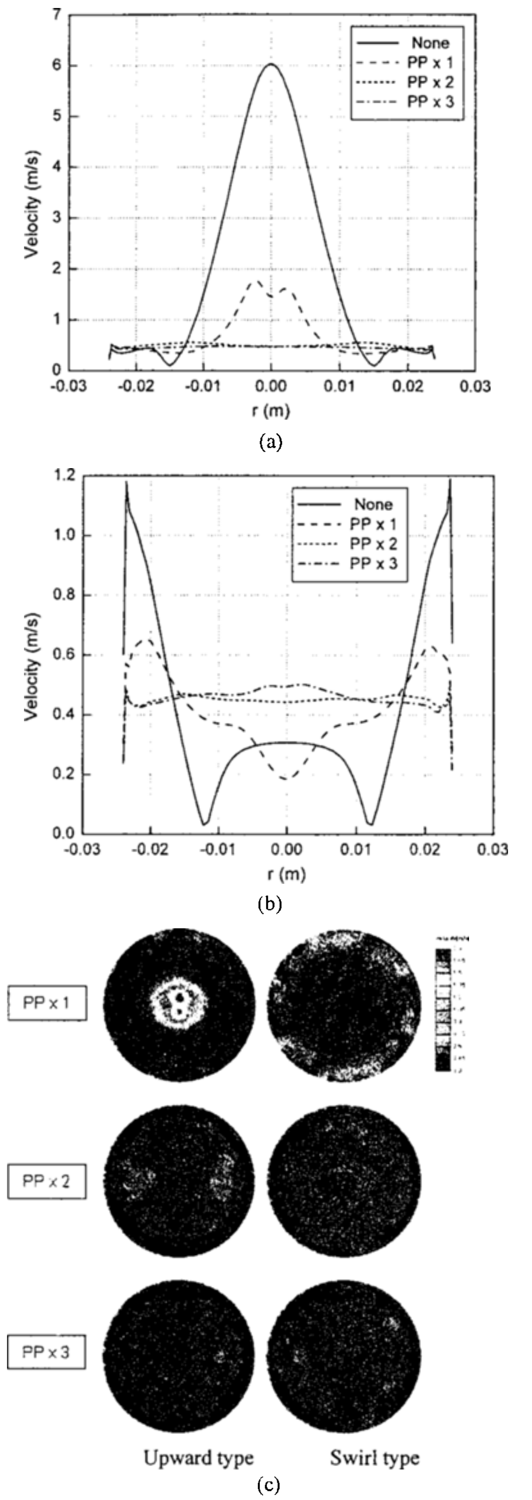
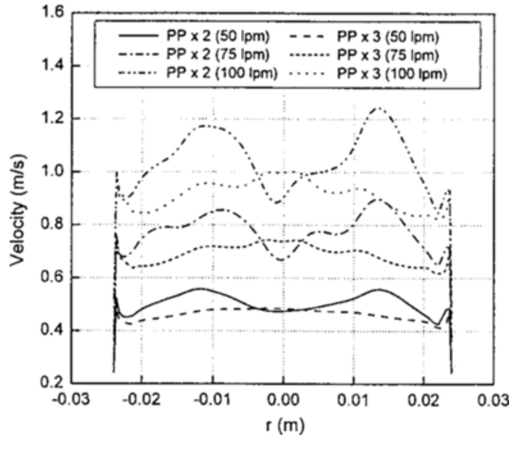
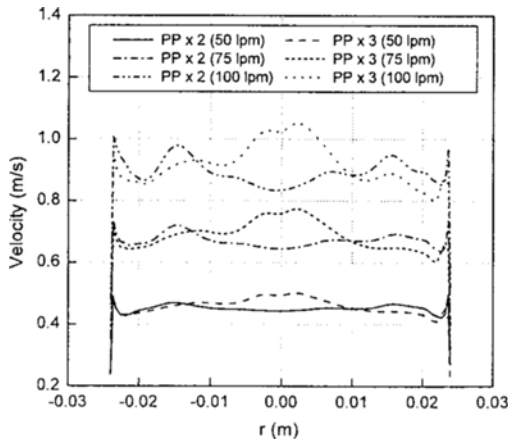


Fig. 6. Effect of the number of the perforated plates with porous area of 10.6% on the velocity: (a) upward type, (b) swirl type, and (c) velocity contours at the honeycomb monolith outlet.



(a)



(b)

Fig. 7. Effects of number of perforated plates and volume flow rate on the velocity profile: (a) upward type and (b) swirl type.

than 2, it can be found that the velocity profile at the outlet of the honeycomb monolith is nearly flat in comparison with the model without the perforated plate. Swirl type cases show similar results as the upward type. In the case where one perforated plate is used, it can be found that the flow is still concentrated near the wall region. The maximum velocity, however, is reduced and the velocity profile becomes more uniform as the number of perforated plates increases. The effects of the number of perforated plates and volume flow rate on the velocity profile are depicted in Fig. 7. In both models of the upward and swirl types, it is shown that the mean velocity at the outlet increases in proportion to the volume flow rate, and the flow uniformity decreases as the volume flow rate increases because a more intensive flow is introduced

Table 3. The mean velocity and standard deviation by increasing the number of perforated plate and volume flow rate for the case of upward type.

Volume Flow Rate	PP x 2		PP x 3	
	Mean V	σ	Mean V	σ
50 lpm	0.50	0.034	0.46	0.021
75 lpm	0.78	0.065	0.69	0.037
100 lpm	1.04	0.106	0.92	0.054

Table 4. The mean velocity and standard deviation by increasing the number of perforated plate and volume flow rate for the case of swirl type.

Volume Flow Rate	PP x 2		PP x 3	
	Mean V	σ	Mean V	σ
50 lpm	0.45	0.012	0.46	0.024
75 lpm	0.67	0.022	0.69	0.045
100 lpm	0.90	0.041	0.92	0.066

with the increase the volume flow rate. Although the flow uniformity decreases as the volume flow rate increases, the standard deviation of the model with perforated plates is less than 0.106, as shown in Table 3, which is very low value compared with that of non-perforated plate model shown in Fig. 4.These results show that the velocity profile of the case with perforated plates becomes more uniform than that of the none-perforated plate model.

In the upward type, when several perforated plates are used, the mean velocity at the outlet increases and the flow uniformity decreases in proportion to volume flow rate supplied. By using the three-perforated plates, however, the mean velocity increases with less reduction of the flow uniformity than that of the model with two perforated plates. The case of the swirl type model in Fig. 7(b), however, shows that the velocity profile with two perforated plates is more uniform than that of the three-perforated plates model. This results from the fact that the perforated plates are installed crosswise to each other and the porous area of the plate is very small (10.6% of total area). When flow passes through the perforated plates, all flow introduced to the plates cannot pass through all the holes of the perforated plates, and therefore, concentrated flow is moved to the lower velocity region and passes through the hole of the perforated plate in that region. For this reason, reverse flow is observed for the case of the model with three perforated plates. This reverse flow is different from the velocity profile of the flow passing through the prior perforated plate.

Tables 3 and 4 represent the mean velocity and standard deviation for the case of upward and swirl types shown in Fig. 7, respectively. In the model with two perforated plates, it can be found that the mean velocity, standard deviation and increment of standard deviation for the case of upward type are larger than those for the case of the swirl type. Therefore, it is concluded that the swirl type is more effective than the upward type with respect to the enhancement of flow uniformity. On the other hand, in the model with three perforated plates, it is shown that the mean velocity is the same for both types, and increment of standard deviation of the upward type is lower than that of the swirl type. This result indicates that the upward type is more effective than the swirl type in model with three perforated plates

Finally, it can be concluded that the model with two perforated plates of the swirl type produces the most effective flow characteristics of all models considered in this work based on the comparison of the standard deviation.

5. Conclusion

A numerical simulation is performed to investigate the variation of flow characteristics by changing such various parameters as inlet configuration, porous area of the perforated plate, number of the perforated plates used, and the volume flow rates. Under each condition considered in this work, the uniformity of the flow stream at the entrance of the catalyst section is evaluated and compared. The results show that flow uniformity can be effectively improved by using the well-designed perforated plates. The following summarizes the main conclusions studied in this work.

In both upward and swirl types, the case with a porous area of 10.6% has the most uniform velocity profile.

The velocity profile becomes more uniform as the number of perforated plates increases.

The mean velocity at the outlet increases in proportion to the volume flow rate and the flow uniformity decreases as the volume flow rate increases.

The case of the swirl type with two perforated plates shows the most uniform velocity profile among the cases studied in this work.

The characteristics of the mixing quality and flow uniformity are very important issues. These issues can probably be a subject of future work. The knowledge gained by these works can be used to design and develop a catalytic combustor that can meet the requirements of the fuel cell power plant system.

Acknowledgements

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Nomenclature

k	:	Turbulent kinetic energy
p	:	Pressure, N/m^2
P	:	Mean-strain production
U_i	:	Velocity of the i-component, m/s
δ_{ij}	:	Unit tensor
ε	:	Dissipation rate
μ	:	Viscosity, kg/m-s
ρ	:	Density, kg/m^3
σ	:	Standard deviation
σ_ϕ	:	Turbulent Prandtl/Schmidt number for ϕ

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